TITLE: New pyrimidine derivatives
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AB 5-Nitropyrimidines containing in the 4- or 6-position a ketonylamino or aldehydoamino group are obtained from the 4- or 6-halo analog and the corresponding amino ketone or aldehyde; the NO2 group may be reduced for continuation of the reaction, which then yields 7,8-dihydropteridines (C.A. numbering). 2,6-Dichloro-5-nitro-4-methylpyrimidine 5 in Me2CO 50 and NaHCO3 6 treated over 1.5 hrs. with AcCH2NH2 3 parts yield after filtration and evaporation 2-chloro-4-methyl-5-nitro-6- (acetonylamino)pyrimidine (I), m. 108° (from Et2O, EtOAc, and petr. ether). Likewise, I 9 and Et2NH 5 parts after 12 hrs. in dioxane yield the 2-diethylamino compound, m. 117-18°, which with H over Raney Ni yields 2-diethylamino-4,6-dimethyl-7,8-dihydropteridine, m. 119-21° (from petr. ether). Similarly, 2,6-dichloro-5-nitropyrimidine in Me2CO and NaHCO3 with AcCH2NH2.HCl (II) yield 2-chloro-5-nitro-6-(acetonylamino)pyrimidine (III), m. 129-31° (from petr. ether), which in the cold with Et2NH in dioxane 12 hrs. yields on dilution with H2O 2-diethylamino-5-nitro-6-(acetonylamino)pyrimidine, m. 119° (from EtOAc and petr. ether), while a similar reaction with PhCH2NH2 gave the 2-benzylamino analog, m. 162°. The Et2N derivative over Raney Ni in dioxane gave 2-diethylamino-6-methyl-7,8-dihydropteridine, m. 158° (from MeOH). Similarly, 2-methyl-4,6-dichloro-5-nitropyrimidine and II in Me2CO in the presence of NaHCO3 gave 2-methyl-4-chloro-5-nitro-6- (acetonylamino) pyrimidine, m. 84° (from Et2O-petr. ether). III 10 in dioxane 50 let stand with 8% NH4OH 30 parts gave 2-amino-5-nitro-6-(acetonylamino)pyrimidine, m. 214° (from dioxane), hydrogenated in OHCNMe2 over Raney Ni to 2-amino-6-methyl-7,8-dihydropteridine, decompose above 210°. 2,6-Dichloro-5-nitropyrimidine (IV) 10 and PhCOCH2NH2.HCl 11 parts in Et2O with NaHCO3-H2O gave 2-chloro-5-nitro-6- (phenacylamino)pyrimidine, m. 173° (from EtOAc-petr. ether), which with PhCH2NH2 in dioxane gave the 2-benzylamino analog, m. 189° (from dioxane), hydrogenated to 2-benzylamino-6-phenyl-7,8- dihydropteridine, m. pyrimidine 242° (from dioxane). Similar reaction in the cold of IV and AcCHMeNH2.HCl in Me2CO with NaHCO3 gave 2-chloro-5-nitro-6-(1-acetylethylamino)pyrimidine, m. 101-2° (from EtOAc-petr. ether); H2NCH2CH(OEt)2 in the above reaction gave 2-chloro-5-nitro-6-(2,2-diethoxyethylamino)pyrimidine, oil, which allowed to stand 3 hrs. with Et2NH in dioxane gave 2-diethylamino-5-nitro-6-(2,2- diethoxyethylamino)pyrimidine, m. 50° (from EtOH); a similar reaction with H2NCH2CH(SEt)2 gave 2-chloro-5-nitro-6-[2,2- bis(ethylmercapto)ethylamino]pyrimidine, oil, which with 10% alc. NH3 yielded 2-amino-5-nitro-6-[2,2-bis(ethylmercapto)ethylamino]pyrimidine, m. 169° (from EtOH). 4,6-Dichloro-5-nitropyrimidine 4.9 in Me2CO 45 containing NaHCO3 6.3 and Na2SO4 5 treated with II 2.8 parts over 0.5 hr. and stirred g hrs. gave 4-chloro-5-nitro-6-(acetonylamino)pyrimidine, m. 60-1° (from petr. ether); the starting material, made from the 4,6-di-HO analog by nitration, followed by treatment with POCl3, m. 101-2°.

IT 875819-80-0P, Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)-
RL: PREP (Preparation)
(preparation of)

RN 875819-80-0 ZCAPLUS

CN Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)- (5CI) (CA INDEX NAME)